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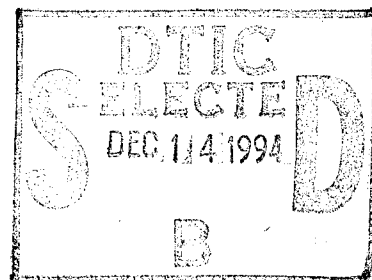
CONTINUED COMPUTATIONAL EVALUATION OF THE  
FEASIBILITY OF NITRATING PRECURSORS TO  $C_{12}N_{12}O_{12}$ .

by

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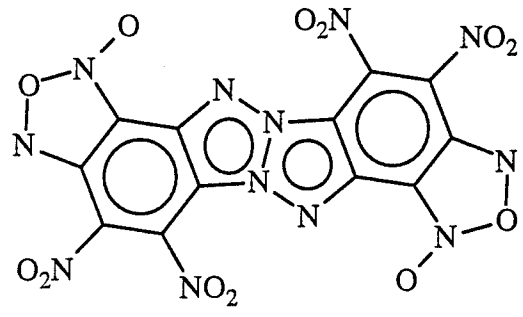


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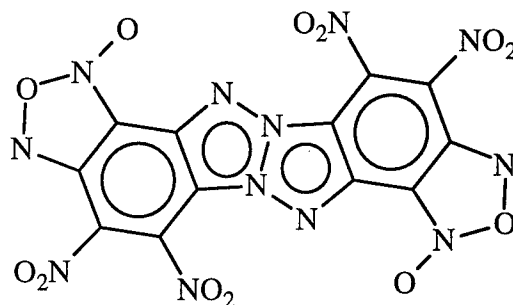
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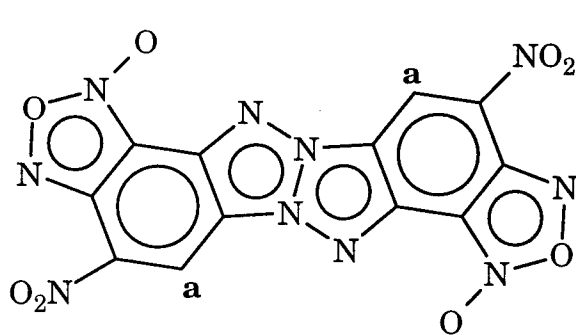
## Introduction

In Technical Report No. 71 (October 20, 1994), we investigated the susceptibility to electrophilic attack involving charge transfer (as in nitration) of several possible precursors to **1**. We computed the average local ionization energies  $\bar{I}_S(r)$  on the surfaces of **2** - **4** (Figure 1) in order to determine the ease of charge transfer at positions **a** and **b**. At the request of M. L. Trudell, we have now extended this study to include **5** and **6**. The procedure used was the same as described in the earlier report, which also discusses the definition and interpretation of  $\bar{I}_S(r)$ . The results are given in Figure 1, together with those obtained previously.

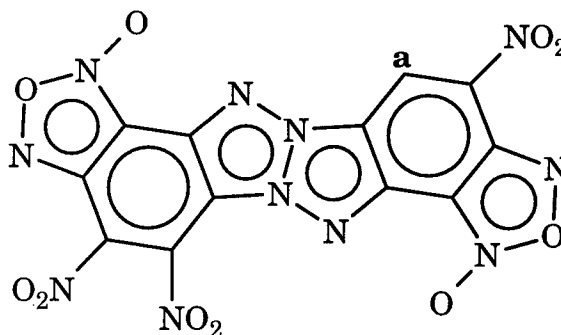


**1**

We find no minimum in  $\bar{I}_S(r)$  at positions **a** in **5** and **6**, which is consistent with what was observed earlier for **4**. This indicates that these are not favorable sites for charge transfer to an electrophile.



**5**



**6**

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